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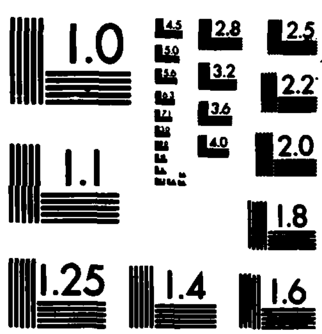

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Report DELNV-TR-0041

EFFECT OF AN UNDERLAYER OF CADMIUM TELLURIDE ON THE REFLECTION-REDUCING PROPERTIES OF ZINC SULFIDE ON MERCURY CADMIUM TELLURIDE

April 1984

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U.S. ARMY ELECTRONICS R&D COMMAND
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For many years ZnS has been used as a passivating coating for HgCdTe photoconductive infrared reflectors. It has served the dual purpose of pasivating the surface and acting as an antireflection coating. A recent suggestion in the Research Division, NVEOL, was to use a layer of CdTe as the first layer on the HgCdTe surface. It was hoped that better passivation might result because of the properties of CdTe. A final layer of ZnS would then be added to achieve further environmental protection and low reflectance.

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The purpose of this report is to investigate, by computational means, the effect of the underlying layer of CdTe on the reflectance-reducing properties of ZnS. This will be done with the absorption coefficient of HgCdTe as a parameter to simulate the effect of cooling the detector to 77°K.

This investigation revealed that the inclusion of a thin (0- to 0.2-micrometer-thick) layer of CdTe under the ZnS coating on HgCdTe not only does not spoil its antireflecting properties but actually improved them somewhat.

Two important features are evident from the computations. When HgCdTe is cooled (k increases), the spectral response of the coating is shifted considerably toward longer wavelengths. In addition, *even if the coating is* designed to provide R_{min} at the proper wavelength when cooled, the reflectance is greatly increased. Both of these effects would adversely affect the performance of HgCdTe as an infrared detector.

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ILLUSTRATIONS

EFFECT OF AN UNDERLAYER OF CADMIUM TELLURIDE ON THE REFLECTION-REDUCING PROPERTIES OF ZINCE SULFIDE ON MERCURY CADMIUM TELLURIDE

I. INTRODUCTION

For many years ZnS has been used as a passivating coating for HgCdTe photoconductive infrared detectors. It has served the dual purpose of passivating the surface and acting as an antireflection coating. A recent suggestion in the Research Division, NVEOL, was to use a layer of CdTe as the first layer on the HgCdTe surface. It is hoped that better passivation might result because of the properties of CdTe. A final layer of ZnS would then be added to achieve further environmental protection and low reflectance.

The purpose of this report is to investigate, by computational means, the effect of the underlying layer of CdTe on the reflection-reducing properties of ZnS. This will be done with the absorption coefficient of HgCdTe as a parameter to simulate the effect of cooling the detector to 77° K.

II. BACKGROUND

Sketches of coating designs considered in this report are shown in Figure 1. The mathematical basis for computing the spectral response of such coatings is discussed in this section.

The reflectance of a surface at normal incidence is given by Eq. 1.

$$R = \frac{(n_o - n)^2 + k^2}{(n_o + n)^2 + k^2} \qquad \text{Eq. (1)}$$

where: n_o = refractive index of incident medium.
$N = n - ik$ = the optical constant of the surface.

The reflectance of a surface similar to HgCdTe is shown in Figure 2, where: $n_o = 1$, $n = 3.9$, and $k = 0$ to 5.

If the surface has a non-absorbing layer deposited onto it, the reflectance, as a function of wavelength, is as given by Eq. 2.

Single and Double Layer Coating Designs

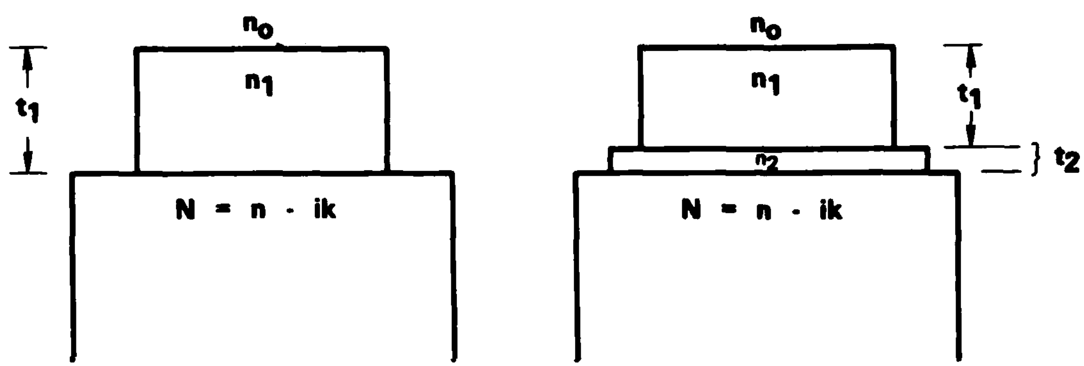

Figure 1. Coating designs and definitions used in this report.

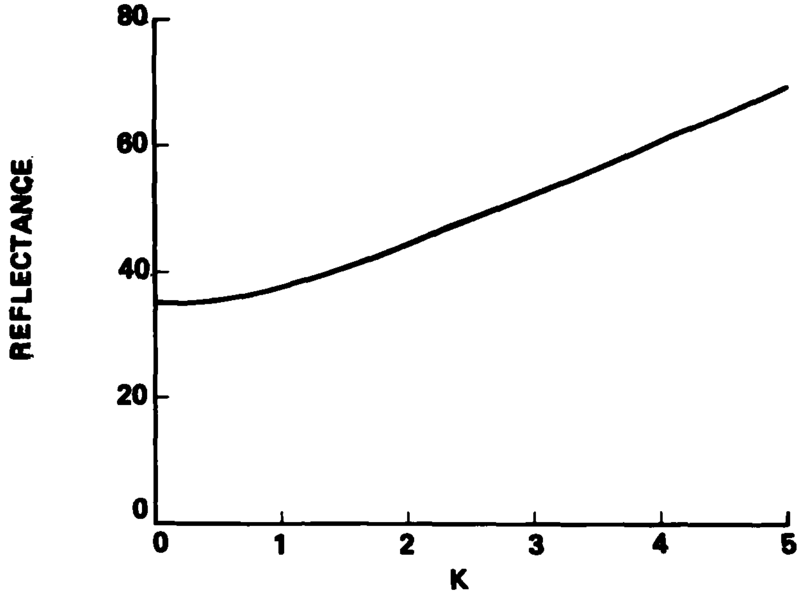

Figure 2. Calculated reflectance of a surface with n = 3.9 and k = 0 to 5.

$$R = \frac{r_1^2 + r_2^2 + 2r_1r_2\,\mathrm{Cos}(2\theta + \delta)}{1 + r_1^2r_2^2 + 2r_1r_2\,\mathrm{Cos}(2\theta + \delta)} \qquad \text{Eq. (2)}$$

where: $\theta = \dfrac{2\pi\, n_1\, t_1}{\lambda}$

$$\mathrm{Tan}\,\delta = \frac{2n_1 k}{n^2 + k^2 - n_1^2}$$

$$r_1 = \frac{n_o - n_1}{n_o + n_1};\; r_2 = \frac{n_1 - n}{n_1 + n}.$$

The minimum reflectance in Eq. 2 occurs when $(2\theta + \delta) = \pi$ (or an odd multiple of π) and is given by Eq. 3.

$$R_{min} = \left(\frac{r_1 - r_2}{1 - r_1r_2}\right)^2. \qquad \text{Eq. (3)}$$

The computed reflectance as a function of wavelength for a simulated layer of ZnS on HgCdTe is shown in Figure 3 with k as a parameter. The thickness of the ZnS was chosen so as to place the R_{min} for $k = 0$ at a wavelength of 10 micrometers. As the value of k changes, the magnitude of the reflectance is greatly affected. The R_{min} moves toward longer wavelengths and the reflectance increases.

The computational approach used here was based on a thin film program developed by Peter Berning.[1]

Eq. 3 can be solved for n_1 or k to give values which result in an R_{min} of zero. The results are given as Eq. 4 and Eq. 5.

$$n_1^2 = n_o\; n + \left(\frac{k^2}{n-n_o}\right). \qquad \text{Eq. (4)}$$

$$k^2 = \frac{(n_on - n_1^2)\,(n_o - n)}{n_o}. \qquad \text{Eq. (5)}$$

[1] Peter H. Berning, "Physics of Thin Films" (Georg Hass, ed.), Vol 1, p 69, Academic Press, New York (1963).

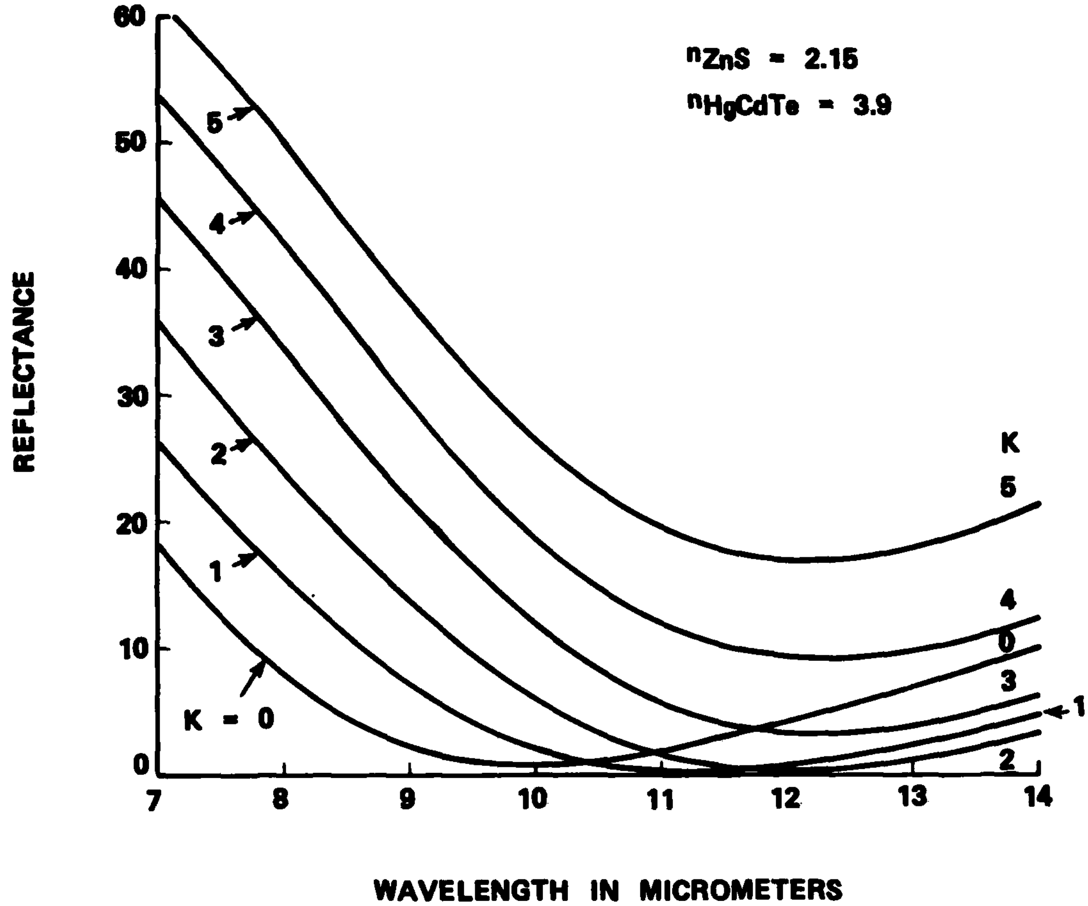

Figure 3. Calculated reflectance as a function of wavelength of ZnS (t = 1.163 micrometer) on HgCdTe with k of HgCdTe as a parameter.

From a previously stated result: $2\theta + \delta = \pi = 4\pi n_1 t_1/\lambda + \delta$ for the first R_{min} to occur. If $\lambda = \lambda_o$ for $\delta = 0$, then one can solve for λ as given in Eq. 6 to find how the minimum is moved by the phase shift, δ.

$$\lambda(R_{min}) = \lambda_o \frac{\pi}{\pi - \delta} . \qquad \text{Eq. (6)}$$

Using Eq. 6 and the expression for Tan δ from Eq. 2, one can calculate the wavelength of R_{min} as a function of k. Results are shown in Figure 4 for ZnS on HgCdTe.

The thickness of the ZnS layer can be adjusted as k is varied so that the R_{min} remains at a wavelength of 10 micrometers. This is shown in Figure 5. Even though the minimum does not shift, the reflectance increases as k increases (except for k = 0 to 2 where it first decreases and then increases). For the values used in the computations ($n_o = 1$, $n_1 = 2.15$, and $n = 3.9$) the value of k which yields $R_{min} = o$ (calculated from Eq. 5) is $k = 1.45$. A plot of R_{min} as a function of k calculated from Eq. 3 is shown in Figure 6. The refractive index of a layer as a function of k which will yield $R_{min} = 0$ was calculated from Eq. 4 and is plotted in Figure 7. For $k = 0$, a layer of ZnS with an index of 2.15 is a good match, but for $k = 5$, for example, a layer with an index of 3.5 would be needed to produce $R_{min} = 0$.

There is an interesting behavior shown in Figure 4. As k increases, the wavelength for R_{min} goes through a maximum then decreases toward λ_o. If the derivative of Tan δ with respect to k in Eq. 2 is set equal to zero, the following expression for the most shifted wavelength for R_{min} is found:

$$k = \sqrt{n^2 - n_1^2} \quad \text{(most shifted } R_{min}\text{).} \qquad \text{Eq. (7)}$$

For the example of Figure 4 with $n_1 = 2.15$ and $n = 3.9$, the value of k is 3.25. However, even though the R_{min} starts moving back at $k = 3.25$, the reflectance continues to increase as can be seen from Figures 3 and 5.

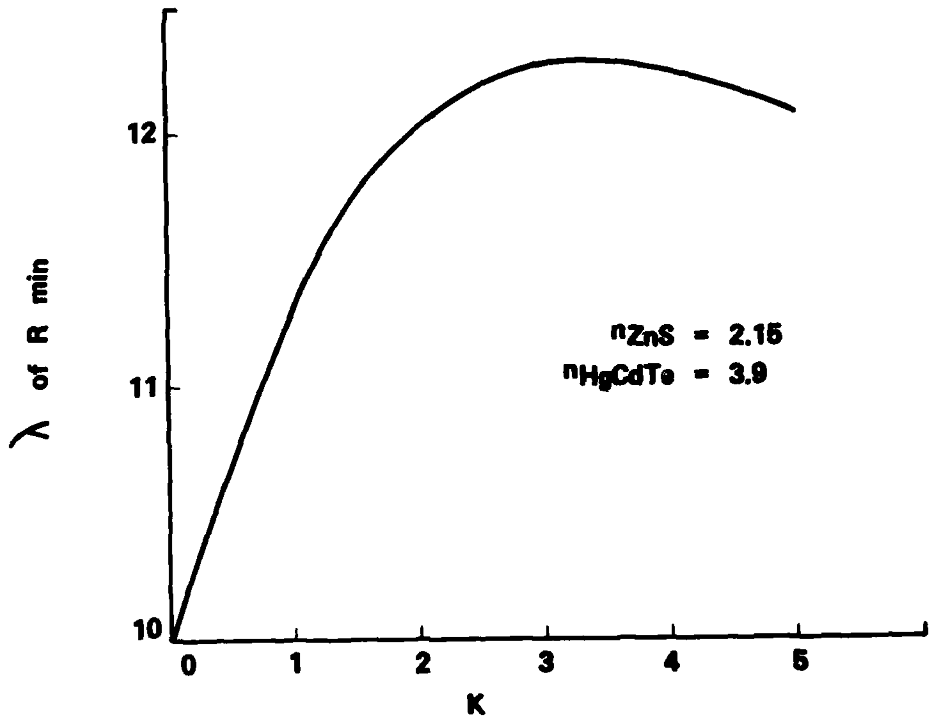

Figure 4. Calculated wavelength of the reflectance minimum of ZnS (t = 1.163 micrometer) on HgCdTe as a function of k of HgCdTe.

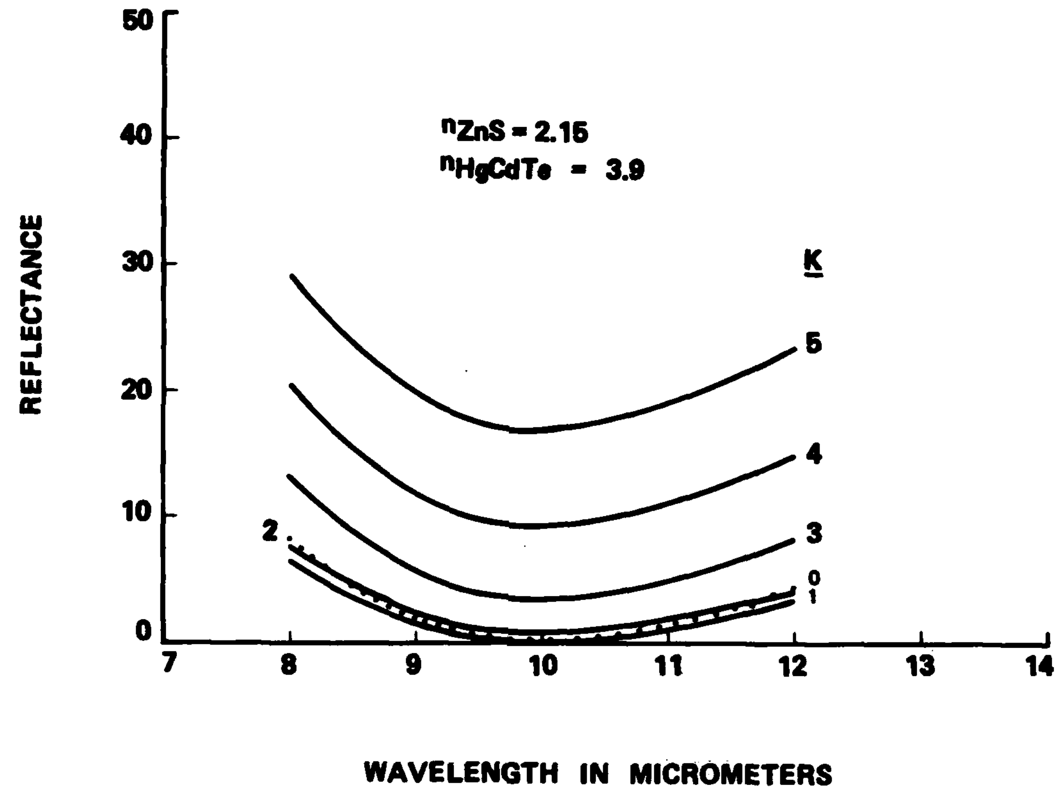

Figure 5. Calculated reflectance as a function of wavelength for ZnS on HgCdTe with k of HgCdTe as a parameter. Thickness of ZnS adjusted to give minimum reflectance at 10 micrometers.

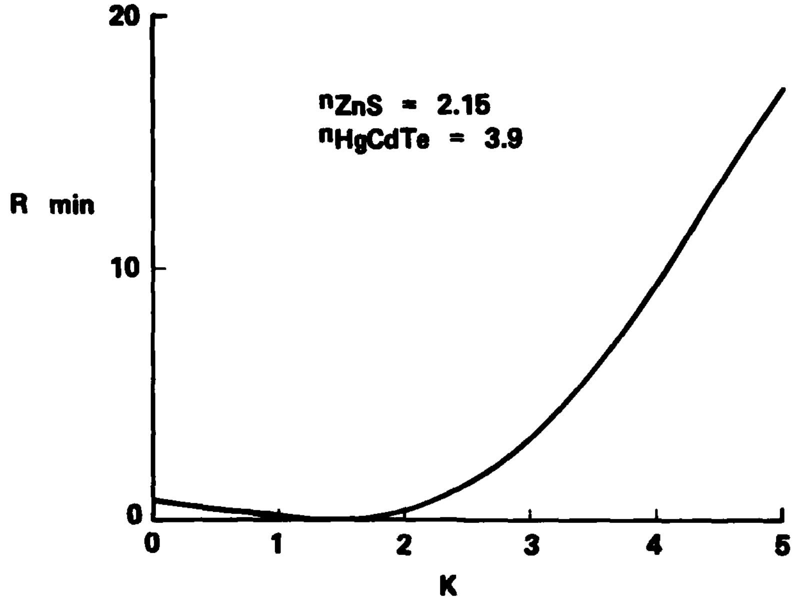

Figure 6. Calculated reflectance minimum as a function of k of HgCdTe for ZnS on HgCdTe.

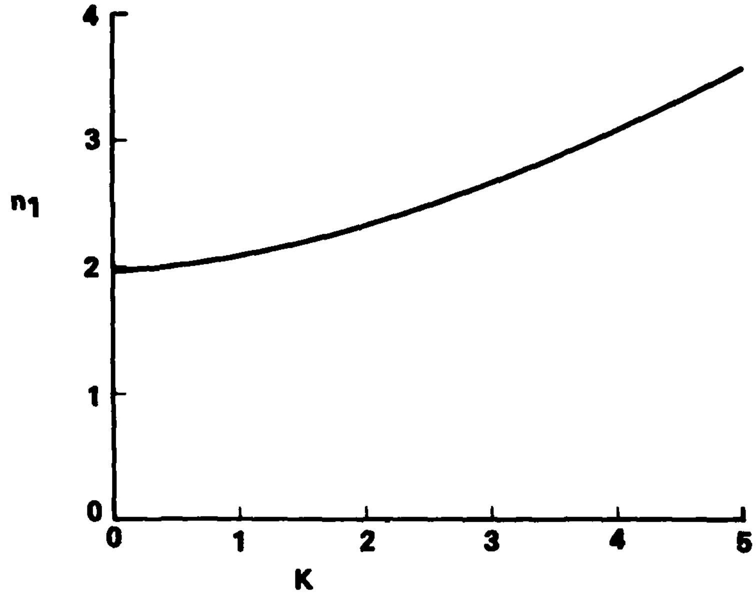

Figure 7. Refractive index of a single transparent layer which can yield zero reflectance on a substrate with n = 3.9 and k = 0 to 5.

III. OPTICAL CONSTANTS OF HgCdTe FROM LITERATURE

In order to put the results presented so far in perspective, reference must be made to measured values of optical constants of HgCdTe presented in the literature. The most recent values found which include measurements at low temperature are those of Finkman and Nemirovsky[2] whose measurements extended into the 8- to 12-micrometer region and down to a temperature of 80° K. These are the only useful results which could be found for HgCdTe at low temperatures. However, even these results are of limited value here because they do not present values of k at 80° K for the region of 8 to 12 micrometers except by extrapolation from values at higher temperatues. This is because their approach required measurement of transmittance, and at 80° K the samples did not transmit sufficiently. The highest absorption constant they could measure was 1000 cm^{-1} which corresponds to a value of k of about 0.1 in the 8- to 12-micrometer region. If an exponential extrapolation is made using their formula, ridiculously high values of k are predicted (more than a million). Therefore, a guess of how high k might be was made by reference to values of Ge below its absorption edge (in the visible to near-infrared regions). Here the value of k has been measured[3] to go above 4.

Therefore, the range of k for simulated HgCdTe was chosen to be from 0 to 5 to correspond to the temperature range from 300° K to 80° K. The value of k may be higher but there is no experimental evidence for it.

IV. COATINGS ON HgCdTe CONTAINING AN UNDERLAYER OF CdTe

Thus far the coatings which have been described have contained only ZnS. When an underlayer of a material such as CdTe is used (thickness of 0.1 or 0.2 micrometer is needed for passivation), the computations become more complicated. In order to design a two-layer coating for which the R_{min} will be at a specified wavelength, such as was the case for ZnS in Figure 5, the thicknesses of both layers must be properly adjusted. A technique was developed some years ago by Cox[4] which does just this. The resulting formula for performing this computation is given as Eq. 8.

$$\mathrm{Tan}2\theta_1 = \frac{-r_3(1 - r_2^2)\,\mathrm{Sin}(2\theta_2 + \delta)}{r_2(1 + r_3^2) + r_3(1 + r_2^2)\,\mathrm{Cos}(2\theta_2 + \delta)} \qquad \text{Eq. (8)}$$

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[2] E. Finkman and Y. Nemirovsky, J. Appl. Phys. *50*, 4356 (1979).

[3] H. R. Philipp and E. A. Taft, Phys. Rev. *113*, 1002 (1959).

[4] J. Thomas Cox and Georg Hass, "Physics of Thin Films" (Georg Hass, ed.), Vol 2, p 262, Academic Press, New York (1964).

where: $\theta_1 = 2\pi\, n_1 t_1/\lambda$

$$\theta_2 = 2\pi\, n_2 t_2/\lambda$$

$$\operatorname{Tan}\delta = \frac{2\, n_2\, k}{n^2 + k^2 - n_2^2}$$

$$r_2 = \frac{n_1 - n_2}{n_1 + n_2}; \quad r_3 = \frac{(n_2 - n)^2 + k^2}{(n_2 + n)^2 + k^2}$$

The approach is to choose the CdTe thickness, t_2, so that θ_2 can be computed. Then θ_2 is plugged into Eq. 8 to allow computation of θ_1 from which the appropriate ZnS thickness can be computed. This process must be done for each specific combination of n's and k's chosen. Results of computations using this approach are shown in Figures 8 and 9 for two different thicknesses of CdTe where the wavelength used in Eq. 8 was 10 micrometers. Comparison with Figure 5 shows that the inclusion of the CdTe layer does not increase the reflectance of the coated HgCdTe but even provides somewhat lower reflectance than the ZnS used alone for the higher values of k.

Figures 10 and 11 show the reflectance of the two-layer coatings presented, with t_2 as a parameter and with an expanded ordinate scale. For $k = 0$ the inclusion of CdTe makes no practical difference when the thicknesses of the layers are chosen by means of Eq. 8. Even when $k = 2$, as in Figure 10, the inclusion of the CdTe is seen to help rather than hinder the antireflecting properties of ZnS. Comparison of Figures 5, 8, and 9 shows that this improvement continues for values of k as high as 5, the highest values used in these computations.

V. CONCLUSIONS

It has been shown that the inclusion of a thin (0 to 0.2 micrometer thick) layer of CdTe under the ZnS coating on HgCdTe not only does not spoil its antireflecting properties but actually improves them somewhat.

Two important features are evident from the figures. When HgCdTe is cooled (k increases) the spectral response of the coating is shifted considerably toward longer wavelengths (Figure 3). In addition, even if the coating is designed to provide R_{min} at the proper wavelength when cooled (Figure 5), the reflectance is greatly increased. If k actually becomes larger than five, which has not yet been shown experimentally, the reflectance would rise much higher than shown in Figure 5. Futher experimental data are needed on the optical properties of HgCdTe at low temperatures for the 8- to 12-micrometer wavelength region before an accurate prediction can be made on how high the reflectance will rise.

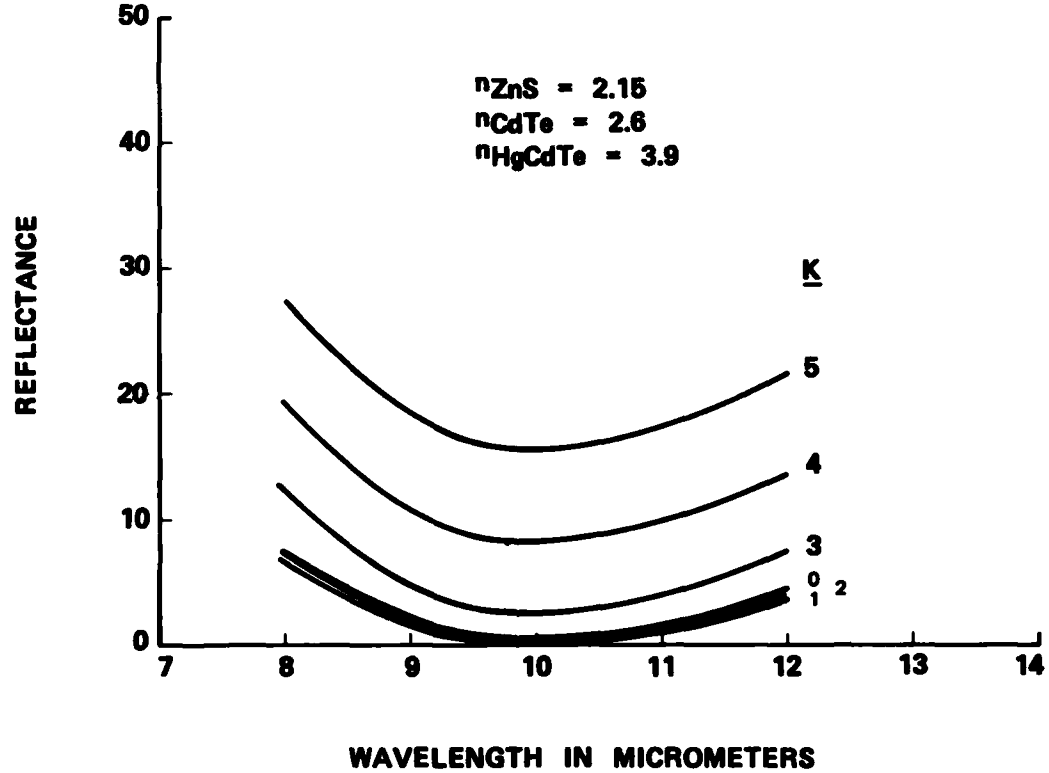

Figure 8. Calculated reflectance as a function of wavelength for HgCdTe + CdTe + ZnS. Thickness of CdTe = 0.1 micrometer. Thickness of ZnS adjusted to give reflectance minimum at 10 micrometers.

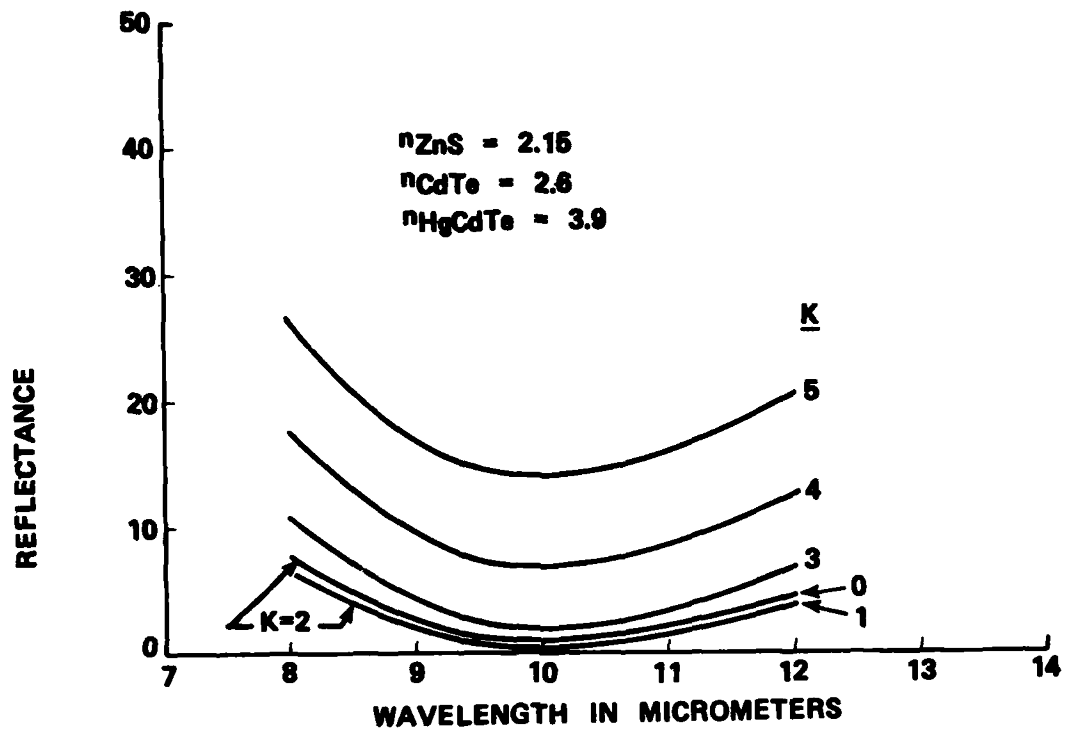

Figure 9. Calculated reflectance as a function of wavelength for HgCdTe + CdTe + ZnS. Thickness of CdTe = 0.2 micrometer. Thickness of ZnS adjusted to give reflectance minimum at 10 micrometers.

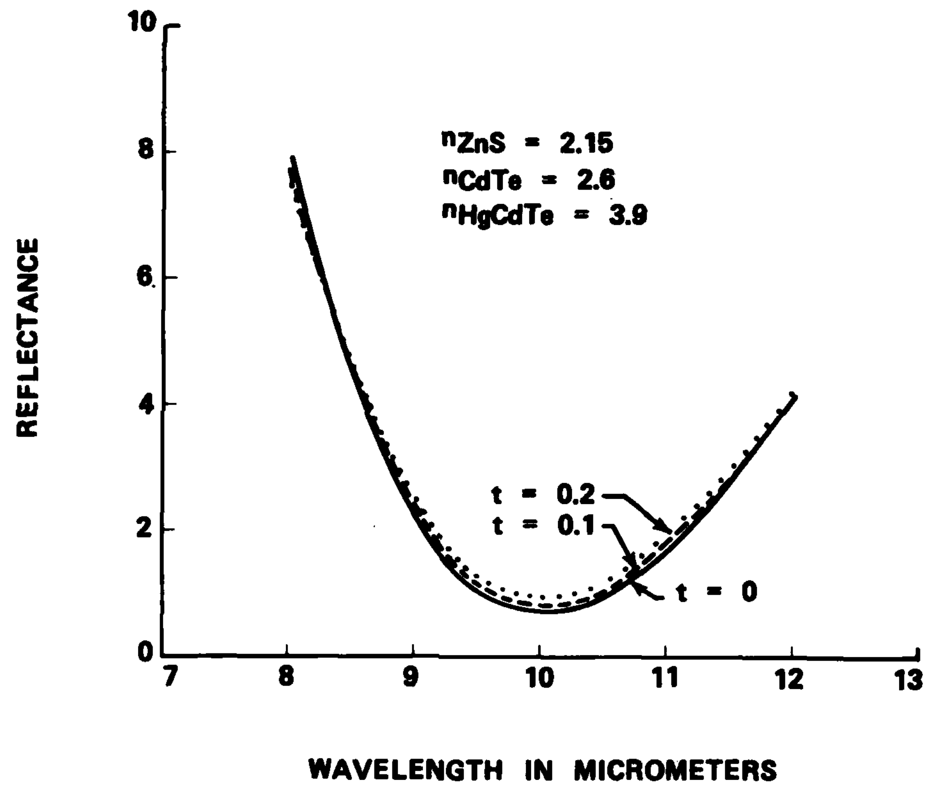

Figure 10. Calculated reflectance as a function of wavelength for HgCdTe + CdTe + ZnS. Thickness of CdTe = 0, 0.1, and 0.2 micrometer. Thickness of ZnS adjusted to give reflectance minimum at 10 micrometers. k of HgCdTe = 0.

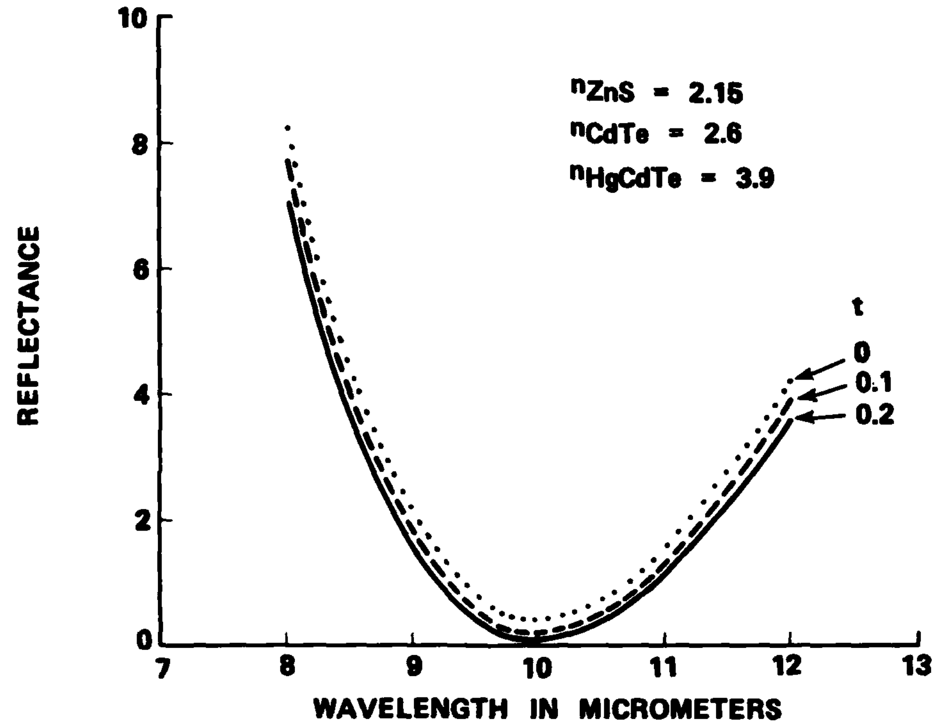

Figure 11. Calculated reflectance as a function of wavelength for HgCdTe + CdTe +ZnS. Thickness of CdTe = 0, 0.1, and 0.2 micrometer. Thickness of ZnS adjusted to give reflectance minimum at 10 micrometers. k of HgCdTe = 2.

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